Effects of impurity on the electronic states in graphite

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に温度差をもち、流れが一次元的になつているとして除いた。この結果Jは $J=J^K+\lambda J^V$ の形に書ける。ここで J^K は、ハミルトニアンのharmonicな項（相互作用のないフォノン系を記述する項）から生ずる流れである。J^V はanharmonicな相互作用があるため生ずる流れで、λ^2 のオーダーまで計算しようとするとこの J^V からの寄与も計算する必要があることが分る。このようにして、harmonicな流れ J^K が、相互作用によつて変化を受ける効果ばかりでなく、anharmonicity によつて生ずる流れ J^V が関係する効果も計算した。

具体的な計算は、Éliashberg[2] のやつたやり方を使つて行つた。J^K と J^V の相関からの寄与を L^{KV} と表わすことにすると、L^{KK}, L^{KV}, L^{VK} は、Normal process に対しても小さな、Umklapp process に対して大きい寄与を与え、定性的によいのであるが、L^{VV} は、このような性質を持たない。Pierls 理論との対応は、今調べているところであるが、L^{VV} は対応がつかないようである。

(1) R. Kubo, M. Yokota, S. Nakajima, J. Phys. Soc. Japan 12 1203 (1957)

(2) G. M. Eliashberg, JETP 14 886 (1962)

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Recently, some experimental results have been repoted for a graphite with dilutely-doped borons; g-shifts, Hall effects, and de Haas-van Alphen effects. Though they have not been accumulated enough to suggest a systematic view about the effect of impurities on the graphite, they moti-

vate us to start a theoretical investigation on this problem. Since there are no theories which consider the effects of impurity on the electronic states in graphite, we calculate the change in electronic states due to an imprity by using a simple two-dimensional model for graphite crystals. Following the Koster and Slater's method in the Wannier's representation, the phase shift of wave functions caused by impurities is investigated. It is concluded that there are one virtual state in the conduction band and one localized state below the valence band if an impurity atom makes an attractive potential field which is strongly localized. Further we investigate the change in the states density as a function of energies in π-band which is caused by the scattering of electrons by the field of impurities. The case, in which potential extends over many lattice sites, is also studied on the basis of effective mass approach. It is found that one cannot expect an energy-dependent change in density of states in both conduction and valence bands as far as one confines with the first order perturbation treatment. In this treatment we obtain the very small phase shift.